4-ISOPROPYL-3-METHYLPHENOL

Other names:	1-Hydroxy-3-methyl-4-isopropylbenzene
	3-methyl-4-isopropylphenol
	4-Isopropyl-5-methylphenol
	4-Isopropyl-m-cresol
	Biosol
	Phenol, 3-methyl-4-(1-methylethyl)-
	o-Cymen-5-ol
	p-Thymol
Inchi:	InChI=1S/C10H14O/c1-7(2)10-5-4-9(11)6-8(10)3/h4-7,11H,1-3H3
InchiKey:	IJALWSVNUBBQRA-UHFFFAOYSA-N
Formula:	C10H14O
SMILES:	Cc1cc(O)ccc1C(C)C
Mol. weight [g/mol]:	150.22
CAS:	3228-02-2

Physical Properties

Property code	Value	Unit	Source
chs	-5648.00	kJ/mol	NIST Webbook
hf	-184.00	kJ/mol	NIST Webbook
hfs	-290.00	kJ/mol	NIST Webbook
hfus	17.57	kJ/mol	Joback Method
hsub	104.40	kJ/mol	NIST Webbook
hsub	106.00	kJ/mol	NIST Webbook
hvap	76.35	kJ/mol	Cheméo Relay (1.0)
ie	8.14	eV	Cheméo Relay (1.0)
log10ws	-2.44		Cheméo Relay (1.0)
logp	2.824		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	3439.94	kPa	Joback Method
rinpol	1332.20		NIST Webbook
rinpol	1334.00		NIST Webbook
rinpol	1336.90		NIST Webbook
rinpol	1332.20		NIST Webbook
tb	511.15 ± 3.00	K	NIST Webbook
tb	519.15 ± 4.00	K	NIST Webbook
tb	511.15 ± 3.00	K	NIST Webbook
tb	511.15 ± 4.00	K	NIST Webbook

tc	731.61	K	Cheméo Relay (1.0)
tf	385.65 ± 2.00	K	NIST Webbook
tf	387.15 ± 2.00	K	NIST Webbook
tf	385.15 ± 2.00	K	NIST Webbook
tf	384.15 ± 2.00	K	NIST Webbook
tf	384.75 ± 2.00	K	NIST Webbook
tf	385.65 ± 2.00	K	NIST Webbook
tf	387.15 ± 2.00	K	NIST Webbook
tf	387.15 ± 2.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.65	J/mol×K	540.04	Joback Method
cpg	325.50	J/mol×K	577.45	Joback Method
cpg	338.45	J/mol×K	614.86	Joback Method
cpg	350.56	J/mol×K	652.28	Joback Method
cpg	361.90	J/mol×K	689.69	Joback Method
cpg	372.56	J/mol×K	727.10	Joback Method
cpg	382.61	J/mol×K	764.51	Joback Method
dvisc	0.0035167	Pa×s	338.12	Joback Method
dvisc	0.0012767	Pa×s	371.77	Joback Method
dvisc	0.0005484	Pa×s	405.43	Joback Method
dvisc	0.0002681	Pa×s	439.08	Joback Method
dvisc	0.0001452	Pa×s	472.73	Joback Method
dvisc	0.0000853	Pa×s	506.39	Joback Method
dvisc	0.0000535	Pa×s	540.04	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54655e+01
Coeff. B	-4.63032e+03
Coeff. C	-8.29300e+01
Temperature range (K), min.	388.00
Temperature range (K), max.	538.94

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3228022&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point